

Phase Transition in IrTe₂ induced by spin-orbit coupling

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IrTe₂ has been renewed as an interesting system showing competing phenomenon between a questionable density-wave transition near 270 K followed by superconductivity with doping of high atomic number materials. Higher atomic numbers of Te and Ir supports strong spin-orbital coupling in this system. Using dynamical mean field theory with LDA band structure I have introduced Rashba spin orbit coupling in this system to get the interpretation for anomalous resistivity and related transition in this system. While no considerable changes are observed in DMFT results of Ir-5d band other than orbital selective pseudogap ‘pinned’ to Fermi level, Te-p band shows a van Hove singularity at the Fermi level except low temperature. Finally I discuss the implications of these results in theoretical understanding of ordering in IrTe₂.

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I. INTRODUCTION

Transition-metal compounds are found to have interesting physical properties such as spin-charge-orbital density waves,[1, 2] superconductivity[3–5] at moderate to low temperature, unconventional transport and magnetism[6]. Most of these properties are believed to be originated from the topology of multiband Fermi surfaces[7] of the parent compound. The multi-orbital transition-metal oxides and chalcogenides exhibit metal-insulator transitions in presence of density wave orders induced instability in the Fermi surface [8]. Also five 3d orbitals of Fe play an important role in magnetism and superconductivity (SC) of Fe pnictides[9, 10] and chalcogenides like SC ordering in LaFeAsO_{1-x}F_x [11, 12]. Along with this “quantum fluctuation” is another parameter which introduce novel electronic states near zero temperature [13]. Failure of the Fermi liquid theory at magnetic quantum critical points (QCPs) in itinerant magnets[14], transition-metal oxides[15], chalcogenides and heavy fermion systems[16] are examples of the extant variety of quantum fluctuations. Transition-metal compounds with geometrically frustrated lattice structure, such as triangular lattices, which often form a ordered low temperature valence-bond solid (VBS)[17] indeed show quantum fluctuation [18].

Recently, interplay between superconductivity and distortion in lattice structure in a transition metal dichalcogenide IrTe₂ of 1T structure have been noticed [19, 20]. It exhibits a phase transition at 270 K from the trigonal (P3m-1) to the monoclinic (C2/m) structure associated with related changes in electrical resistivity and magnetic susceptibility [21]. In addition superconductivity can also be found in this compound substituting Ir of the parent compound by Pt[22] or Pd [23]. Both IrTe₂ and PtTe₂ have trigonal CdI₂-type structure and belong to the space group P3m-1 but Pt is having higher atomic number than Ir. High atomic number can be related to strong spin orbit (SO) coupling because it is directly proportional to the fourth power of atomic number. So the superconducting order in doped IrTe₂ is likely to be re-

lated to the spin orbit coupling. While undoped IrTe₂ manifests a first order phase transition whereas PtTe₂ shows no anomaly down to lowest temperatures.

In 1T-IrTe₂ the transition metal Ir layers and chalcogen Te layer are bound to each other by interlayer van der Waals attraction with each of these layers forming a triangular lattice[24]. So the transition metal ions are having three equivalent transition metal bonds. The phase transition in IrTe₂ can be identified by an abrupt change in electrical resistivity and as well as a sudden decrease in Pauli paramagnetic susceptibility. Charge-orbital density order is predicted in IrTe₂ at moderate to high temperature which results in structural transition [24]. Though a density wave transition is envisaged[24], experiments manifest that one side of the triangular Ir lattice is changed uniformly whereas the other two Ir-Ir bonds remains same after the transition [19]. Moreover the parent chalcogenides (IrTe₂ and PtTe₂) shows no sign of superconductivity down to lowest experimentally measured temperature[25, 26]. Due to large atomic number of Ir, the transition in the compound IrTe₂ is related with large SO coupling. Large SO coupling sometimes cause magnetic anisotropy and multiferroicity[27]. Furthermore it can lead to unconventional superconductivity[28] in topological superconductors. Complete understanding of the electronic properties of IrTe₂ needs the explanation of structural phase transition.

Analysis of the extant experimental review speculates that IrTe₂ with large SO coupling unveils almost bad metallic feature throughout all the temperature[21]. The most intriguing phenomena is its phase transition near 270 K with anomaly in resistivity and magnetic susceptibility[21]. The nature of this phenomena is still under debate. The existence of superconductivity with doping of Pd or Pt in association with disappearance of 270 K phase transition is another interesting phenomena in the phase diagram[19]. The phase diagram of IrTe₂ shows a huge resemblance with high T_c cuprates and some heavy fermion superconductors[29]. The magnetic quantum critical point (QCP) is close to the superconductivity which gives the evidence of existence of

a QCP of charge-orbital density wave nearer to the superconducting order and this density wave ordering may give rise to the superconducting order [30]. Parent IrTe₂ shows multiband nature in its effective Fermi surface. Further modification of only one Ir-Ir bond [19] at the ordering temperature opposes the charge-orbital density wave order. Briefly all properties of IrTe₂ show strong correlation throughout all the temperature and doping, so dynamical mean field theory (DMFT) [31, 32] will be the best way to explain the unconventional ordering in it. In this paper I present a full DMFT calculation of IrTe₂ to predict the electronic properties of the system closer to the transition temperature region.

Tight binding band structure of IrTe₂ is calculated by using Ir-5d and Te-5p bands which gives two bands crossing Fermi energy level. Primarily these are the hybridized bands of Ir-5d and Te-5p orbitals. Although there is mixing of d and p orbital, Te-5p orbitals are playing dominant character in the bands near Fermi energy. LDA band structure calculation also predict the same. In Fig.1 I show the noninteracting band structure, corresponding density of states and Fermi surface map (in $\Gamma - M - K - \Gamma$ plane and $A - L - H - A$ plane) of the bands nearest to the Fermi level. Band structure of IrTe₂ (Fig.1a) clearly manifests the existence of negative indirect band gap. Six Fermi surface (FS) pockets can be seen from the LDA FS in Fig.1b. The lower band is crossing Fermi level along $\Gamma - M$ direction closer to Γ point, originated mainly from the Te-5p_x and Te-5p_y orbitals and is almost fully filled while in the other band dominant contribution comes from Te-5p_z and Ir-5d bands. The upper band is more spreaded and crosses Fermi level at higher momentum. Our band structure and FS calculation closely tracks the earlier results [24].

For IrTe₂, a two-band Hubbard model is mandated by LCAO results, and adequate treatment of dynamical correlations underlying bad metallic behavior is achieved by dynamical-mean field theory. DMFT approaches are proven to be successful in treating strong dynamical fluctuations in correlated electronic systems [1, 13, 33–35] which made them useful tool of choice in the context of correlated electrons. The two band Hubbard model I used is (denoting lower band (Te-p) as ‘a’ and upper band (Ir-d) as ‘b’) $H_{el} = \sum_{k,l,m,\sigma} (t_k^{lm} + \epsilon_l \delta_{lm}) c_{kl\sigma}^\dagger c_{km\sigma} + U \sum_{i,l=a,b} n_{il\uparrow} n_{il\downarrow} + U_{lm} \sum_i n_{il} n_{im}$. where l and m run over both band indices a and b. The intra-orbital correlation is taken as U and U_{ab} is the inter-orbital correlation which play a major role throughout. Due to large atomic number of Ir inter-orbital hopping is negligible in comparison to spin orbit interaction. Moreover due to large spin-orbital coupling Rashba effect is an important addition to the two band Hubbard Hamiltonian. The Rashba Hamiltonian is $H_R = \alpha \sum_{k,\sigma,\sigma'} (\sigma \times p) \cdot \hat{z} c_{kl\sigma}^\dagger c_{kl\sigma'}$. where α is coefficient of Rashba coupling, p is momentum and σ is the Pauli matrix vector. To solve full Hamiltonian $H = H_{el} + H_{Rashba}$ within DMFT I have combined the multi-orbital iterated perturbation theory (MOIPT) for H_{el} [36] with a momentum-dependent modification to

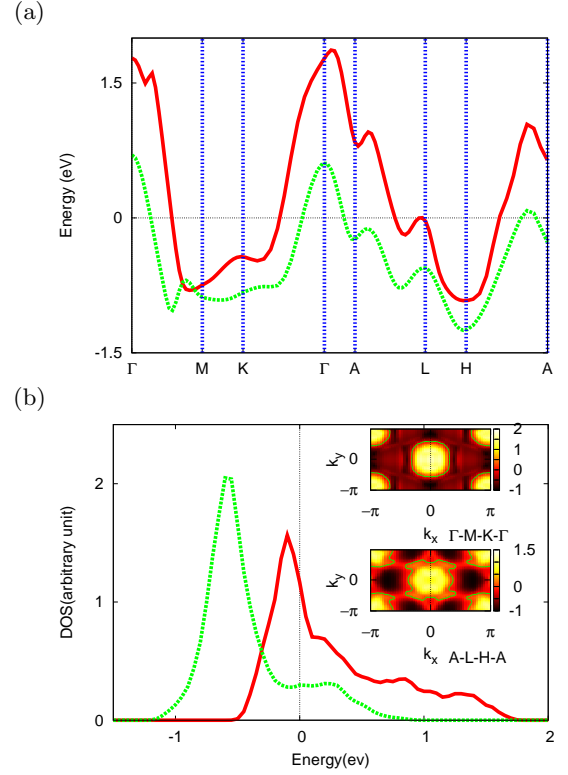


FIG. 1: (Color Online) (a) Ir-5d (red line) and Te-5p (Green line) bandstructure and (b) density of states near Fermi level. Fermi surface of IrTe₂ at two plane (inset of Fig.1b). Upper inset is for the Γ -M-K- Γ plane and lower inset is for A-L-H-A plane.

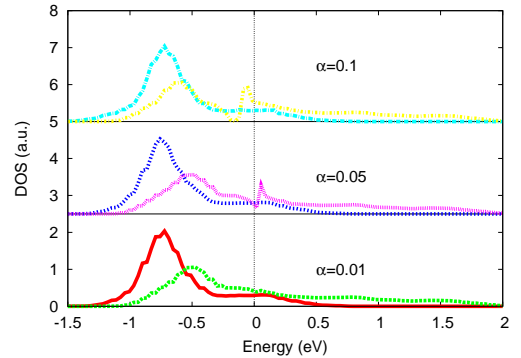


FIG. 2: (Color Online) Density of states near transition temperature (transition temperature is noted here for the temperature where resistivity shows peak value and around which hysteresis is observed) for different value of the coefficient of spin orbit coupling.

include Rashba coupling. The ordered state and physical observables are calculated self consistently from DMFT in presence of an infinitesimal symmetry breaking due to SO coupling. Following earlier procedure [1], I will compute DMFT spectral functions and transport properties in the normal state and ordered state.

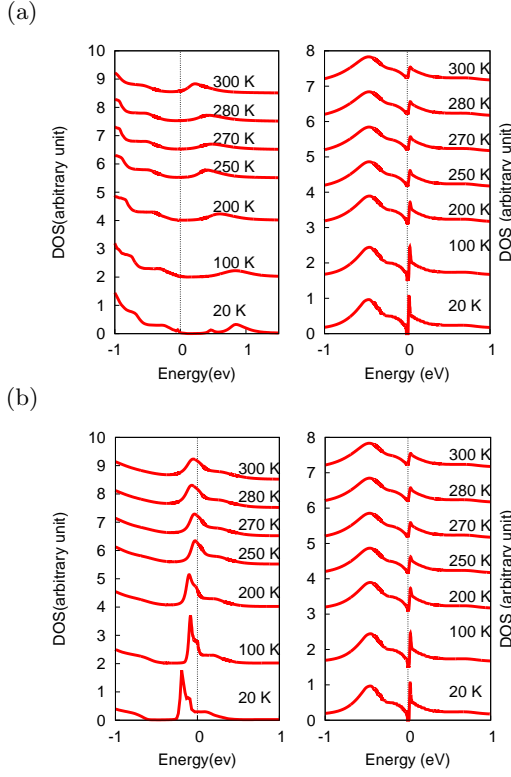


FIG. 3: (Color Online) T -dependent density of states for (a) temperature increasing from 0 K to 300 K, (b) temperature decreasing from 300 K to 0 K. Left panel is for Te-5p band and right panel is for Ir-5d band.

I now show how the approach predicted above explains a wide variety of physical responses noticeable in IrTe₂. The DMFT many body density of states for different value of α is shown in Fig.2. I observe that with increasing value of α a pseudogap like behavior is emerging in the density of states near Fermi level, which in turn proves the role of spin orbit coupling in ordered state of IrTe₂. Without the presence of spin orbit interaction the transition related changes is not observed in its theoretical spectra. As displayed in Fig.2 the spectral function exhibits a prominent orbital selective pseudogap for small value of α which confirms the presence of SO interaction tuned ordering in the system near 270 K. Since the ordering can be found experimentally also I will take $\alpha = 0.05$ in further calculation. Moreover materials with partially filled t_{2g} levels, like IrTe₂ also, charge degree of freedom is coupled with the orbital one, resulting in Peierls instability induced density wave. Presence of these type of density wave transition can also be found here.

Now the DMFT spectral function for the Ir-d (a band) and Te-p (b band) bands is given in Fig.3a with increasing temperature and in Fig.3b with decreasing temperature and corresponding self energies in Figs.4a, 4b, 4c and 4d. Both the spectral functions with increasing temperature exhibits a ‘peak’ near Fermi energy at lower temperature and a pseudogap like feature at Fermi en-

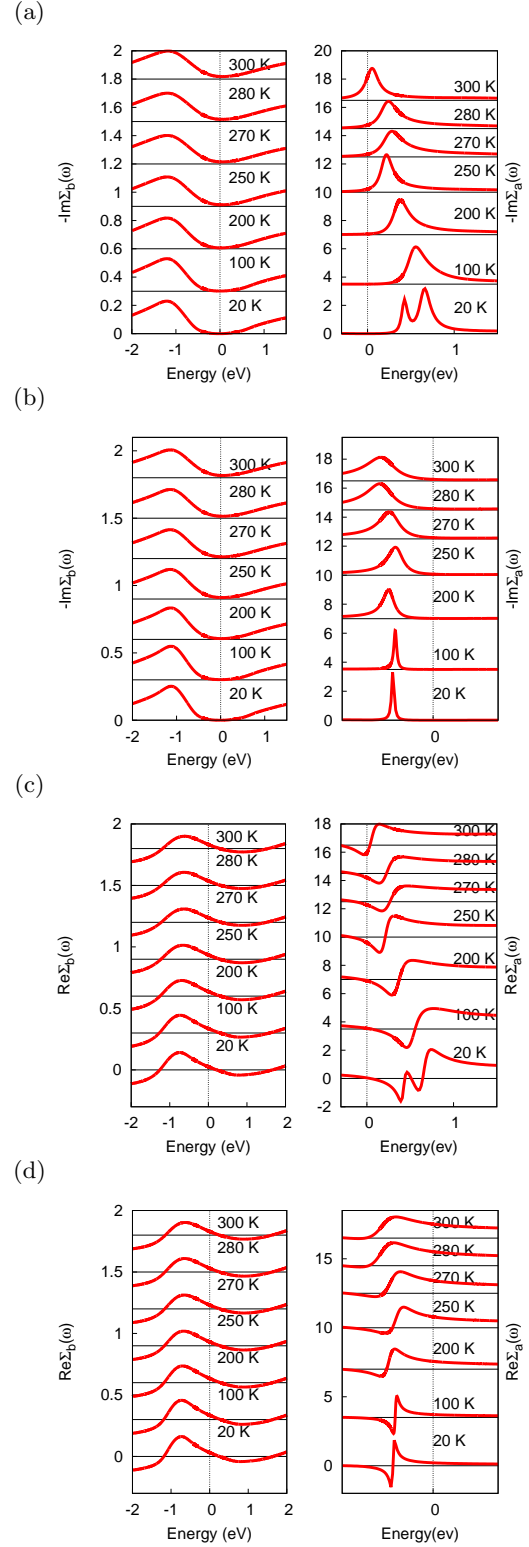


FIG. 4: (Color Online) T -dependent imaginary part of self energy when (a) temperature increasing from 0 K to 300 K, (b) temperature decreasing from 300 K to 0 K.

T -dependent real part of self energy when (c) temperature increasing from 0 K to 300 K, (d) temperature decreasing from 300 K to 0 K.

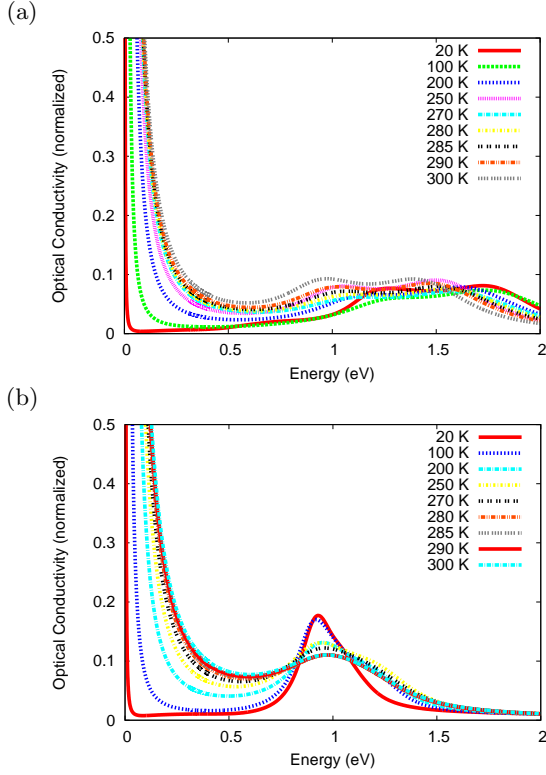


FIG. 5: (Color Online) DMFT results for T -dependent optical conductivity when (a) temperature increasing from 0 K to 300 K, (b) temperature decreasing from 300 K to 0 K.

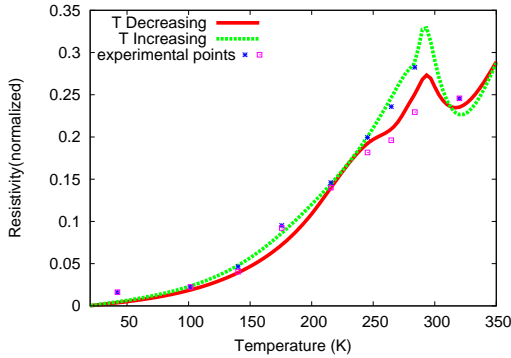


FIG. 6: (Color Online) Temperature dependent DMFT resistivity for temperature increasing and decreasing. DMFT results manifests good agreement with previous experimental results (represented by two types of points for temperature increasing and decreasing after A. F. Fang et al.[21]).

ergy for both the bands. For the ‘a’ band a broad peak comes closer to the Fermi level with increasing temperature whereas the peak remains pinned near Fermi level for the ‘b’ band. However with decreasing temperature a sharp “polelike” feature near Fermi energy is spotted in ‘b’ band closer to the Fermi level in almost similar

fashion as earlier but in the other band the sharp pole is observed exactly at the Fermi level unlike the earlier one. This sharp feature is originated due to the finite value of α so it may be argued that the ‘pole’ structure along with the low energy pseudogap is a result of SO coupling. I further find that the sharp pole in the spectral function is a van Hove singularity which disappears at low temperature. The remarkable shift of the peak from the Fermi level reduces the kinetic energy of electrons which may be the driving force of the transition. However due to the presence of pseudogap this dichalcogenide shows bad metallic behavior throughout.

Interestingly the self energies prove the non Fermi liquid behavior ($\text{Im } \Sigma(0) > 0$) exactly at the 250 K temperature above which the anomaly in the resistivity can be found. The panels on the left show Ir-5d band self energies while the right panels are for Te-5p self energies. The imaginary part of self energies are shown in Fig.4a and in Fig.4b for both the bands with increasing and decreasing temperature. A careful scrutiny of the imaginary part of self energy for ‘a’ band with increasing temperature till 300 K shows a prominent pole in the energy range of 0.2 eV i.e. very near to Fermi level. Now this pole remains on Fermi level at temperature near 270 K, same as the temperature where resistivity shows a jump. Particularly from this temperature onwards $\text{Im } \Sigma_a(0)$ shows a nonzero value. The finding of nFL (non Fermi liquid) behavior in self energy beyond 250 K persist till high temperature. But throughout all the temperature the other band shows no such important changes. It exhibits incoherent Fermi liquid ($\propto -\omega^2$). Surprisingly with decreasing temperature imaginary part of ‘a’ band self energy exhibits a different type of behaviour. A peak is observed throughout the temperature region which is completely below the Fermi level though the peak in the self energy varies with temperature. The peak comes closer to the Fermi level near 250 K where the resistivity shows an exception. Peak-width also varies with temperature. It decreases and ceases to almost a single line at lower temperature. Real part of the self energies (with increasing and decreasing temperature) also exhibits same type of behavior. While the ‘b’ band self energy (both imaginary and real part) remains almost featureless, the other band shows a good variation with temperature and gives a clue to hysteresis in resistivity. With increasing temperature the peak in self energy is above Fermi energy and then comes towards Fermi energy and finally it crosses Fermi level while with decreasing temperature it is below Fermi level with peak position changing with temperature and coming nearest to Fermi level near 250 K. The results support that the Rashba spin-orbit coupling associated with inter-orbital coulomb interaction has a remarkable effect on the temperature dependent self energy and density of states. It is observed that near 250 K self energy and spectral function are changing their weight on Fermi level to show singularity. This is exactly that temperature where the resistivity shows a sudden departure.

Now to support the prediction of Rashba SO coupling

DMFT result should explain transport as well. In DMFT, this calculation is simplified: it is an excellent approximation to compute transport co-efficients directly from the DMFT propagators [38], since (irreducible) vertex corrections rigorously vanish for one-band models, and turn out to be surprisingly small even for the multi-band case. In Fig.5 I present the DMFT optical conductivity as a function of T . A reflection of pseudogap at low T is found which closes rapidly with increasing T . The optical conductivity with increasing temperature is shown in Fig.5a. It shows a featureless broad peak at high energy upto 1.5 eV with a Drude like peak at low energy. Both of the Drude peak and broad peak decreases with increasing temperature with large spectral weight transfer to higher energies. Since I have kept only two bands nearest to the Fermi energy in LCAO calculation, agreement at higher energies is not expected. Since the self energy shows nFL behavior the peak at zero energy can be explained as a reflection of reduced incoherence in the ordered state at low temperature. Moreover a broad peaklike structure can also be found in earlier experiments[21]. Optical conductivity with decreasing temperature is shown in Fig.5b. In contrast to the earlier one a sharp peak is observed in optical conductivity at 1.0 eV which is sharper at lower temperature and the peak height also decreases with increase in temperature and becomes broader. This change in peak is directly coming from the Rashba SO coupling. Such a temperature dependence of optical conductivity over a wide energy region is quite unconventional and reminiscent of phase transition in the system. Clean orbital selective singularity found to be set in with decreasing temperature via rapid spectral weight transfer. This type of pseudogap is a precursor to density wave in this system. The overall change in the optical conductivity points out the ordering to set in the system. Here also the zero energy relatively sharp peak is found which also decreases significantly with the temperature and reflects the reduced incoherence in optical conductivity with lowering temperatures.

Fig.6 shows the temperature dependent DMFT resistivity of IrTe_2 . Consistent with previous experimental[21] and theoretical reports [24] pure IrTe_2 exhibits a hysteresis in resistivity. With increasing temperature resistivity shows a peak near about 280 K and with decreasing temperature resistivity shows a peak at about 270 K which agrees well also with earlier experiments[21]. It shows a sudden increase in resistivity upon cooling. The resistivity shows bad metallic nature without any anomaly upto lowest temperature below this hysteresis region. The bad metallic nature can be explained as opening of pseudogap alongside a van Hove singularity at Fermi level. Since the resistivity reflects bad metal so the consequent short scattering mean free path makes quasiclassical Boltzmann equation based transport calculation invalid and in this regime DMFT should fit best. This bad metallic behavior below hysteresis region is due to reduction of the strong normal state scattering. This type of behavior in

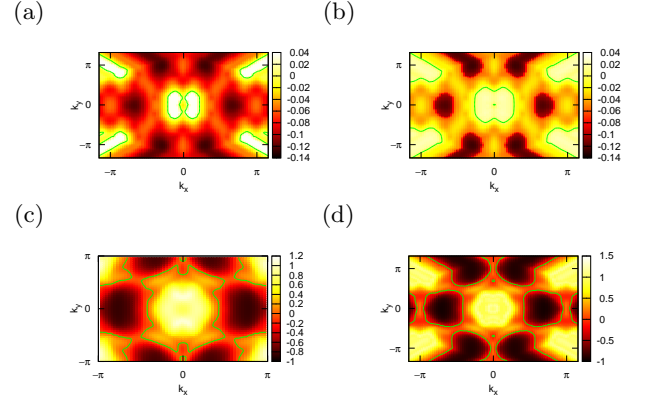


FIG. 7: (Color Online) DMFT FS spectra for Γ -M-K- Γ and A-L-H-A direction at temperature 20 K ((a) and (c)) and at 290 K ((b) and (d)) while temperature is increasing.

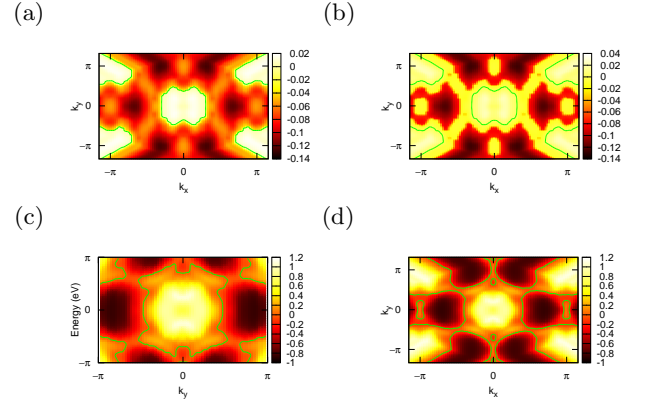


FIG. 8: (Color Online) DMFT FS spectra for Γ -M-K- Γ and A-L-H-A direction at temperature 20 K ((a) and (c)) and at 290 K ((b) and (d)) while temperature is decreasing.

resistivity is reminiscent of structural transition. Thus the transport and spectral properties undergoes very good accord with experiments which supports the proposal of Rashba spin orbit coupling in IrTe_2 . If the Rashba spin orbit coupling alternative is the cause for this phase transition then the one particle spectral function and renormalized band dispersion will also give the proof for same. DMFT FS spectra along A-L-H-A direction are also shown (Fig.7 and Fig. 8) to see the change in three dimensional FS map for temperature increasing and decreasing. Our DMFT FS spectra are consistent with the earlier results [22]. In low temperature near 20 K the FS spectra (Fig.7a and Fig.8a) shows almost same behavior while at higher temperature the FS spectra becomes different. At 290 K it shows different map though the symmetry remains same. The FS maps are calculated along the Γ -M-K- Γ and A-L-H-A direction of the Brillouin zone (BZ). Ir-Ir (Ir-Te) bond in the crystal structure corresponds to the A-L (A-H) direction. The

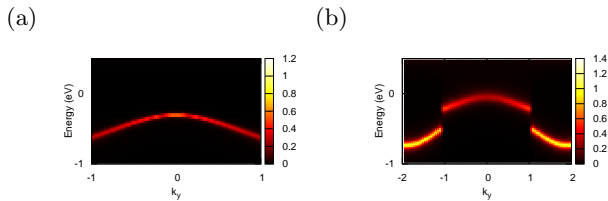


FIG. 9: (Color Online) Theoretical ARPES map along H-L-H direction at (a) low temperature (20 K) and (b) high temperature (290 K). Zero energy along y-axis represent Fermi level.

centre of the BZ corresponds to Γ point ($k_z=0$) or A point ($k_z \sim 0.8\pi$). At high temperature due to thermal excitations relatively large Fermi pockets can be seen (Fig.8c). This sizable high-T spreading of FS is due to non zero value of self energy at $\omega = 0$. The flower-shaped Fermi surface is consistent with the earlier calculation[22, 37]. Along A-L-H-A direction six connected beads can also be identified in the FS map at 290 K which seems to be smeared out at low temperature. It is noteworthy that the FS map at 20 K, well below the transition temperature (shown in Fig.7a, b, Fig.8a and b) is appreciably showing almost same structure. In contrast the Fermi pockets which are observed at higher temperature are vanished at low-T FS map. So across the 270 K ordering transition the contour of the FS does not change significantly while the Fermi pockets change dramatically at low temperature. This vanishing of pockets are observed perpendicular to the A-H (Ir-Te bond) direction. Therefore it can be concluded that both of the orbitals (Ir 5d and Te 5p) are involved in this ordering and the transition can be called as a charge-orbital ordered state. Further a closer scrutiny of the DMFT results show that the central pocket around Γ point has developed an elongated shape instead of an hexagonal shape as in LDA results. I believe that this important modification arises due to an orbital dependent electronic structure reconstruction that is developed from the spin orbital coupling factor. It can be noted that three dimensional Fermi surface of IrTe₂ reveals rich dispersions reflecting the importance of layered electronic structure. This result exactly goes with the previous theoretical and experimental band structure results, where, the change in FS is proposed as change in crystal structure [39] due to the ordering below 270 K. Thus such a qualitative agreement between the DMFT results based on SO coupling and earlier theoretical and

experimental FS in details gives a credibility of the theory.

However to give further evidence of SO coupling induced pseudogap the same formulation must also describe ARPES as well. I now consider the DMFT ARPES maps of band-structure along L-H direction in the Brillouin zone at both high and low temperature. The dramatic change in the FS is vanishing of Fermi pockets at low temperature. To demonstrate this I compare the band dispersions along L-H direction at 20 K (Fig.9a) and 290 K (Fig.9b). It is found that while the band crosses Fermi level at 290 K forming the FS pockets, it is well below Fermi level at 20 K leading to a energy gap. This gap is not found everywhere in the FS so in the spectral function also there is presence of pseudogap. This specifies that the change in FS arises from a relocation of the band which also allows a ordering transition. Now this related band that forms the pockets is mainly dominated by Te-p orbitals. As observed in Fig. 3a, the Te-p DOS exhibits a distinct peak located at Fermi level at higher temperature and the peak shifts from Fermi level at lower temperature. The energy shift of Te-p band from Fermi level alongwith a pseudogap ‘pinned’ to Fermi level of Ir-d band reduces the spectral weight at Fermi energy and so the energy of the electrons also decreases significantly, which further drives a phase transition in the system.

In conclusion, these results show that all the important physical responses in IrTe₂ and the density wave type transition are associated with the van Hove singularity and pseudogap at Fermi level. The bands near Fermi level are strongly reallocated forming a pseudogap and on the other hand removing van Hove singularity from the Fermi energy. This pseudogap is also reflected in optical conductivity which also gives a clear manifestation of interband transition due to Rashba spin-orbit coupling. Optical conductivity also shows that carrier number reduction due to spin orbit coupling is less than the reduction of incoherent scattering. However the steep jump in resistivity at transition temperature is also related with nFL behavior due to the pseudogap at the Fermi level. Finally the FS and ARPES also supports the pseudogap nature at a particular direction of Brillouin zone. This suggests that the charge and orbital degree of freedom is coupled to drive the system into a ordering transition. This findings also have further important implications on a broader level for the systems with partially filled t_{2g} level and large SO coupling.

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